Use and Misuse of Reflectors

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DISCLAIMER

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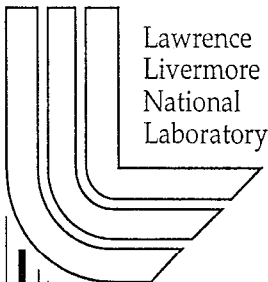
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Use and Misuse of Reflectors

Overview

Reflectors can be very useful if used properly, but can lead to completely incorrect answers if misused. The difference between use and misuse of reflectors can be very subtle and sometimes hard to understand. Therefore it is important for you to understand how to use reflectors, and at the same time, avoid misuse of reflectors.

Physically when can Reflectors be Used?

Reflectors can be used in problems that have a symmetry. For example, you may be able to simplify your input preparation by only describing 1/8-th of a system and using reflecting planes. It is physically acceptable to do this ONLY in the following situations,
1) Only planes can be used. No other surfaces can preserve the required reflection properties so that both sides of the surface are mirror reflections of one another.
2) Only place plane reflectors at positions of symmetry, so that a particle reflecting from the plane moves in the same relative direction that it would have moved if it were allowed to cross the plane.
3) Only use reflectors if the resulting shape can fill the entire space without overlap or leaving holes. Note, only planes can do this; quadratic surfaces, such as cylinders, cones, spheres. etc., cannot do this.

What's the Advantage of Reflectors?

Some users have the mistaken idea that the advantage of reflectors is that by making the geometric description of a problem simpler their problem will run faster. Generally this isn't true. The real advantage of reflectors is that their use can minimize the amount of input preparation that users must do. A secondary consideration is that using reflectors may simplify the geometry to the point where it is easier for users to interpret and understand results.

Misuse of Reflectors

It is surprising how often people misuse reflectors. Classic examples are where users use quadratic surfaces as reflectors to imply a symmetry that does not really exist in a problem. Here's a few examples,

1) A repeating hexagonal lattice of fuel elements surrounded by water. This can be properly replaced by one cell using six reflecting plane boundaries, e.g., see the below hexagonal example input. However, this cannot be replaced by a cylinder (a quadratic surface) with the same overall volume as the hexagonal cell. This should be obvious, since a series of cylinders cannot fill all space without overlap and/or holes. So it is surprising how often users make the mistake of assuming this can be done.
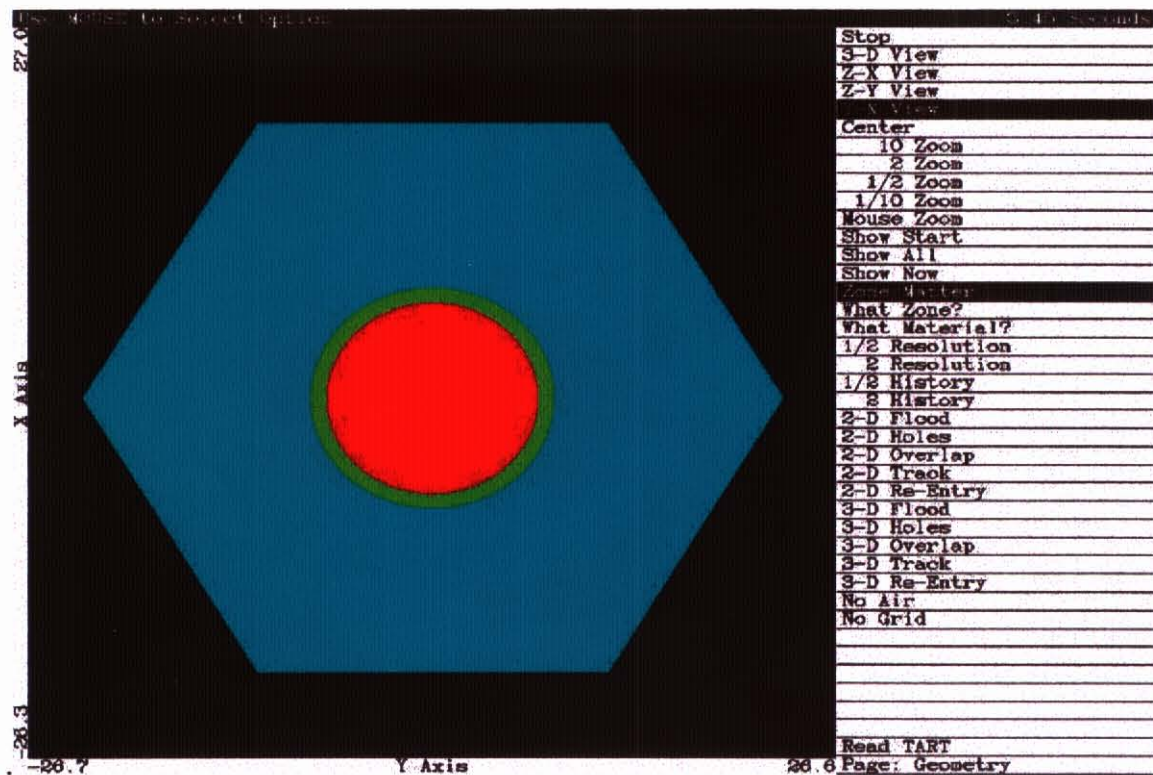
2) A spherical system with beams ports on the x, y, and z axis in the positive and negative directions, i.e., a total of six beam ports, e.g., see the below spherical example input. This can be replaced by 1/8 of the system using x, y, and z plane reflectors. This can also be replaced by 1/6 of the system using rotated planes to define a rectangular cone (like a pyramid). However, this cannot be replaced by 1/6 of the system using a circular cone (a quadratic surface). Again, this should be obvious, since a series of circular cones cannot fill an entire sphere without overlap and/or holes. So again, it is surprising how often users make the mistake of assuming that this can be done.
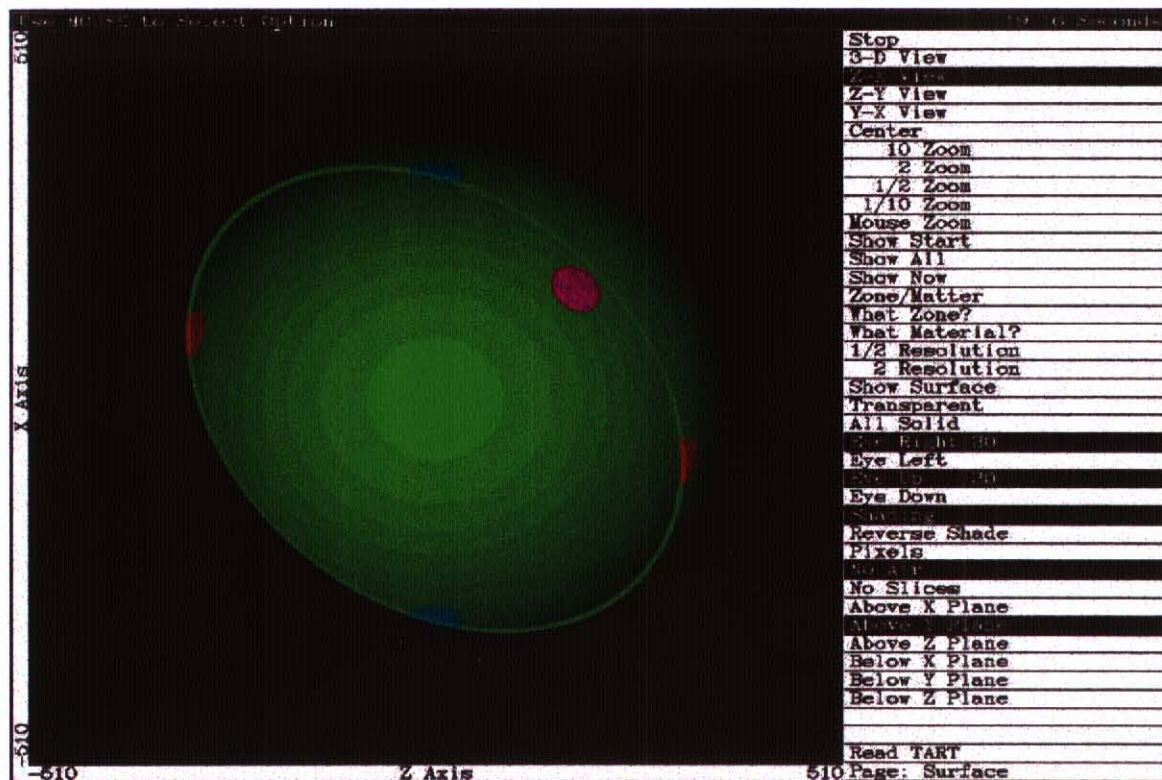
Both of the above examples of the misuse of reflectors can be subtle and hard to understand. It sounds like a cylindrical representation of the hexagonal array of fuel cells is reasonable. It also sounds like a circular conic section representation of spherical symmetry is reasonable. If you think strictly in terms of volumes these do indeed seem like reasonable representations. But if we consider the direction of transport, in fact in both of these examples the quadratic reflector will bias the results. Particles reflecting off of the cylinder do not follow the same trajectory as particles in the hexagonal fuel cells. Similarly particles reflecting off the circular cone do not follow the same trajectory as particles in the spherically symmetric system. Using these quadratic reflectors biases the trajectory of the particles, which can very significantly change the answers from their true values.

We can see this effect below. On the left is the a square repeating lattice. On the right is a cylindrical approximation to the square lattice, where the radius of the cylinders is defined so that both square and cylinder representation have the same volume. Now consider that in each case we replace the repeating lattice by one cell and reflecting surfaces. On the left only the center square is used, surrounded by four reflecting planes. On the right only the center cylinder is used, where the cylinder itself is reflecting.

Now consider a neutron emitted at the center of each cell travelling outward toward the reflecting boundary. On the left we can see that if the neutron reflects off of the bounding plane it ends up moving in the same relative direction as if it has been allowed to pass through the plane, i.e., in this case the trajectory is not biased. In contrast, on the right we can see that ALL neutrons emitted at the center are traveling in a direction orthogonal to the surface of the reflecting cylinder. Therefore when these neutrons reflect off of the bounding cylinder they are reflected back along their path, directly toward the origin, i.e., in this case the trajectory of the particles is biased toward the center of the cylinder.
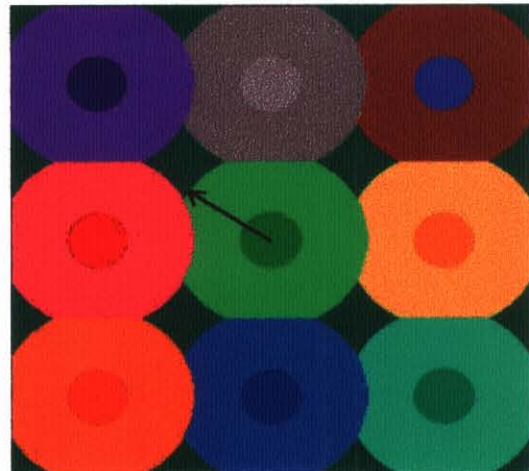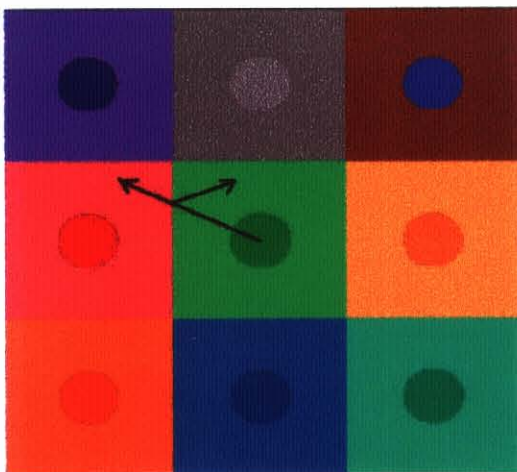

Even without considering the subtle difference in trajectories, problems of misuse of reflectors could have been avoided in the above described problems simply by observing that in these cases there is no real spatial symmetric about either the cylinder in the case

of the hexagonal cell, or the cone in the case of the spherical system. In general there simply cannot be the required symmetry on two sides of any quadratic surface; only planes can be used to correctly model reflecting images of geometry.

You can also make a mistake even when using only planes, if you do not remember to place reflecting planes ONLY at positions of symmetry. For example, consider a simple infinitely repeating planar system of a layer of fuel followed by a layer of water infinitely repeated. The only positions of symmetry in this system are at the centerline of each fuel and water layer.
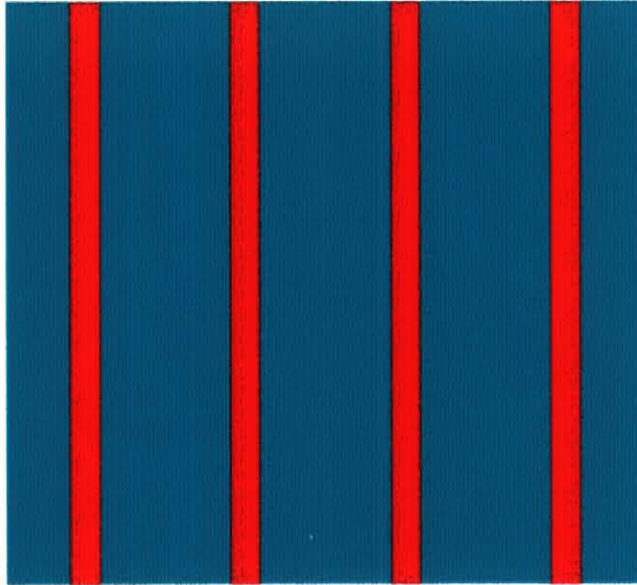
You can replace this by 1/2 a cell by placing a reflecting plane at the centerline of a layer of fuel and a second reflecting plane at the centerline of the next layer of water. Or you can replace this by an entire cell by placing a reflecting plane at the centerline of a layer of water and another reflecting plane at the centerline of the next layer of water. Note, in both of these cases the geometry is symmetric about the reflecting planes. However, you cannot replace this by a reflecting plane at the edge of a layer of water and a second reflecting plane at the edge of the next layer of water. This would also include a complete cell, but the reflecting planes would not be at positions of symmetry. Indeed if you did this any calculation would think that your geometry really was symmetric about these planes and the cell would appear to be twice as wide as it really is

Centered 1/2Cell - o.k   Centered Full Cell - o.k.   Non-Centered Full Cell - bad

Note how in the above three figures the geometry really is symmetric about the left and right edges of the first and second figures, but it is not really symmetric about the third, rightmost, figure. This third figure infers that the cell is symmetric about these boundaries, making the cell appear to be twice its true width.

How Important is This Effect?

The magnitude of the bias introduced by using quadratic reflectors depends on how smooth the flux is, both in space and direction. When the flux is very smooth the effect of the bias will be minimized. However, when the flux is varying rapidly in space and is highly directed the effect can be very large.

The worst case will be when the flux is highly directed and there is a lot of reflection of this highly directed flux, which then accentuates the bias introduced by the circular conic reflector. Here's an example problem where the effect is maximized due to streaming of particles and lots of reflection.

Geometry: a 500 cm radius sphere centered on the origin, and three 50 cm radius cylinders, one each aligned with the x, y, and z directions, and passing through the center of the sphere. This simple situation can be visualized as a 500 cm sphere with six 50 cm circular holes through it, where the holes are on the positive and negative x, y, z axii. Inside of the sphere is void or a very low density material, so there are essentially no interactions within the sphere.

Source: a point, isotropic, 1 MeV monoenergetic, source at the origin.

Question: What fraction of the emitted particles enter the six holes in the sphere.

Answer: In this situation this is a simple geometry problem with an analytical solution. The fraction entering the holes will be the fraction of the area of the holes facing the source to the area of the sphere.

Area of six holes: $6 \text{ pi } R^2 = 6 \text{ pi } [50]^2$
Area of sphere: $4 \text{ pi } R^2 = 4 \text{ pi } [500]^2$
Ratio $= 6 [50]^2 / 4 [500]^2 = 3/200 = 0.015$

It is actually slightly different from this because of the curvature of the face of the cylinder passing through the sphere, but this is close enough for what we are about it do.

Let's now run some Monte Carlo calculations,
1) First run the entire system, and you will find that you do indeed get this answer.
2) Next model 1/8-th of the system by adding reflecting x, y, and z planes, at $x = y = z = 0$, and only transport in the 1/8-th of the system defined by, $x = y = z >= 0$. Again, you will get the right answer, because the use of planes does not bias the results.
3) Finally model 1/6-th of the system using one cylinder aligned with the z axis, and a reflecting circular cone aligned with and on the z axis and 48.19 degrees wide. The inside of this cone corresponds to 1/6-th of the volume of the complete system. With most codes you will have to move the source slightly off center - move it to $z = 0.001$, $x = 0$, $y = 0$. In this case you will find that because of the bias introduced by the cone the fraction entering the holes is **over a factor of 6 too large - that's over 600 % too high**.

In the last case the circular cone is acting like a lens to focus the particles toward the z axis. If you move the source around just a little bit you can completely change the answer, because you are completely changing how the cone focuses the particles. So by moving the source you can get almost any answer you want, and none of these answers corresponds to the answer in the original problem, because there is no lens and focussing in the original problem; this focussing is all nonsense introduced by improperly modeling this system.

What's scary about this is that if you try to verify your answer by using the same geometry, you will get the same answer using any code. For example, I have verified that three different Monte Carlo codes - COG, MCNP, and TART, all give the same **WRONG** answer for the above problem with the conic reflector. So it is the responsibility of the code user - **YOU** - to realize when and how you can use reflectors.

But this is a completely theoretical problem that nobody would actually run, right? No, actually it is very similar to a number of real problems. Indeed what prompted me to write this tutorial on reflection is that users were actually modeling 1/6-th of a system as described above, and using a number of different Monte Carlo codes to verify their answers. As I said: **scary, isn't it!!!!**

Bottom Line: Caveat Emptor, if you use quadratic reflecting surfaces, because your results can be unpredictable. In some cases they may look quite good, in other cases (such as the above example) the answer can be completely wrong.

Defining Reflectors for TART

Let's discuss how reflectors are defined and used to TART,

1) ZONES, not SURFACES, reflect.
2) To define a zone to be reflecting, instead of assigning a material to it using the TART keyword matz, use one of the TART reflector keywords: reflx, refly, reflz, reflgp, reflq. Personally I find these TART keywords misleading since it makes it sounds like a surface (x plane, y plane, z plane, general plane, or quadratic), rather than a zone is reflecting. But this is what I inherited with TART, so we are stuck with these keywords.
3) Only if you want to know how many particles reflected off of each type of surface is it important which TART reflector keyword you use. Otherwise all of these keywords can be used interchangeably, i.e., define your reflecting zones using any or all of the TART keywords: reflx, refly, reflz, reflgp, or reflq.
4) Here's a typical TART input line defining zones 16, 23 and 47 to be reflecting,

reflx 16   23   47

Normally in defining TART input we try to avoid defining spatially overlapping zones; these can complicate the interpretation of results. However, in the case of reflecting zones, we do not expect any particles to enter and score anything in reflecting zones, so you need not be too concerned with overlapping zones. For example, when we model 1/8-th of a spherical system by using reflecting x, y, and z planes, we can,

1) Model 1/8-th as the octant with x >= 0, y >= 0, and z >= 0.
2) We can then model three reflecting zones, 1) x < 0, 2) y < 0, 3) z < 0

and we need not be concerned that the three reflecting zones overlap.

The only reason for trying to eliminate this overlap is that it makes it easier to use TARTCHEK to check for errors, i.e., there could be other overlapping zones in your input that you did not intend.

Interpreting Results

If you properly use reflectors to define only a portion of a system, particles should transport through your partial system exactly the same way they would transport through the entire system. In particular flux and deposition should be exactly the same in either a properly defined portion of a system or the entire system.

The normal TART output is ZONE INTEGRALS for flux, deposition, production, etc.. These will be exactly the same if you properly model a fraction of a system using reflectors, or the entire system.

Where you have to be careful in interpreting results is only when you convert results to per cc or per gram. To do this ALWAYS use the volume of each zone in the entire system, not the portion of the system you model. In this case you have to be careful in

using the TART calculated zone volumes for a portion of a system. For example, if you model 1/8-th of a system using reflectors, TART will calculate the volume of only the zones you have defined, i.e., 1/8-th of the true volume of each zone in the entire system.

Also be aware that TART cannot analytically calculate the volume for all possible shaped zones; when it cannot calculate the volume of a zone in the output the volume is defined to be 1.0. So before using TART calculated volumes to define results per cc or per gram check the TART output report to insure that all of the zone volumes that you need have been properly defined. If they have not, consider using TART's option to statistically sample the volume of oddly shaped zones, see the TART options mcvdisk and mcvplane.

Bottom Line: To correctly interpret results,
1) For INTEGRAL zone results, these will be EXACTLY the same in a portion of a system modeled using reflectors as in an entire system, so that no scaling is required.
2) For results per cc or per gram, use the volume of each zone in the entire system. So be aware that when modeling 1/N-th of a system the TART calculated volume of each zone will be only 1/N-th the volume of the volume in the entire system.
3) For results per cc or per gram, check the TART output to insure that all of the zone volumes that you need have been properly defined.

Hexagonal Example Input

```
name   reflector #1
box  t32
*
* Complete artificial hexagonal cell example
*
critcalc  15   1   3.
xplane  1  20.0
clones  1   2 thru 6
zrotate   60.0  2
zrotate  120.0  3
zrotate  180.0  4
zrotate  240.0  5
zrotate  300.0  6
cylz    7  7.0
cylz    8  8.0
zplane   9 -20.0
zplane  10 20.0
* unused surface - merely to center image for tartchek
cylx    11  40.0
jb  1  7                 -9 10
jb  2 -7 8                 -9 10
jb  3  1 2 3 4 5 6 -8 -9  10
jb  4 -1                 -9 10
jb  5 -2                 -9 10
jb  6 -3                 -9 10
jb  7 -4                 -9 10
jb  8 -5                 -9 10
jb  9 -6                 -9 10
jb 10  9
jb 11 -10
matl  1   18.7  0.55 92235 0.45 92238
matl  2    5.6  1.0 26000
matl  3    1.0  2.0  1001 1.0 8016
matz  1   1
matz  2   2
matz  3   3
reflx  4 5 6 7 8 9 10 11
end
```

Spherical Example Input

```
name   reflector #2
box  t32
*
* Complete artificial spherical example
*
sphere  1  500.
sphere  2  510.
cylx    3  50.
cyly    4  50.
cylz    5  50.
xplane  6   0.
yplane  7   0.
zplane  8   0.
jb 1  -6 -7 -8  1
jb 2  -6 -7 -8 -1  2 -3 -4 -5
jb 3  -6 -7 -8 -1  2  3
jb 4  -6 -7 -8 -1  2  4
jb 5  -6 -7 -8 -1  2  5
jb 6            -2
jb 7  6         2
jb 8  7         2
jb 9  8         2
matl 1    1.6e-7 1.0   7014
matl 2    2.8    1.0  13027
matl 3    5.6    1.0  26000
matz 1  1
matz 2  2
matz 3  3  4  5
reflx 7 8 9
source1   1  0.001 0.001 0.001
end
```

Square Cell Example Input

```
name   reflector #3
box  t32
*
* Complete artificial square cell example
*
critcalc 15  1  3.
xplane  1 -80.0
xplane  2 -40.0
xplane  3   0.0
xplane  4  40.0
xplane  5  80.0
yplane  6 -80.0
yplane  7 -40.0
yplane  8   0.0
yplane  9  40.0
yplane 10  80.0
zplane 11 -20.0
zplane 12  20.0
cylz  13    7.0 -60.0  -60.0
cylz  14    7.0 -60.0  -20.0
cylz  15    7.0 -60.0   20.0
cylz  16    7.0 -60.0   60.0
cylz  17    7.0 -20.0  -60.0
cylz  18    7.0 -20.0  -20.0
cylz  19    7.0 -20.0   20.0
cylz  20    7.0 -20.0   60.0
cylz  21    7.0  20.0  -60.0
cylz  22    7.0  20.0  -20.0
cylz  23    7.0  20.0   20.0
cylz  24    7.0  20.0   60.0
cylz  25    7.0  60.0  -60.0
cylz  26    7.0  60.0  -20.0
cylz  27    7.0  60.0   20.0
cylz  28    7.0  60.0   60.0
* inside cylinders
jb    1   13  -11  12
jb    2   14  -11  12
jb    3   15  -11  12
jb    4   16  -11  12
jb    5   17  -11  12
jb    6   18  -11  12
jb    7   19  -11  12
jb    8   20  -11  12
jb    9   21  -11  12
```

```
jb    10    22   -11  12
jb    11    23   -11  12
jb    12    24   -11  12
jb    13    25   -11  12
jb    14    26   -11  12
jb    15    27   -11  12
jb    16    28   -11  12
* inside square, outside cylinders
jb    17   -13   -11  12  -1  2 -6  7
jb    18   -14   -11  12  -1  2 -7  8
jb    19   -15   -11  12  -1  2 -8  9
jb    20   -16   -11  12  -1  2 -9 10
jb    21   -17   -11  12  -2  3 -6  7
jb    22   -18   -11  12  -2  3 -7  8
jb    23   -19   -11  12  -2  3 -8  9
jb    24   -20   -11  12  -2  3 -9 10
jb    25   -21   -11  12  -3  4 -6  7
jb    26   -22   -11  12  -3  4 -7  8
jb    27   -23   -11  12  -3  4 -8  9
jb    28   -24   -11  12  -3  4 -9 10
jb    29   -25   -11  12  -4  5 -6  7
jb    30   -26   -11  12  -4  5 -7  8
jb    31   -27   -11  12  -4  5 -8  9
jb    32   -28   -11  12  -4  5 -9 10
* outside world
jb    33     1
jb    34    -5
jb    35     6
jb    36   -10
jb    37    11
jb    38   -12
matl  1   18.7  0.52 92235 0.48 92238
matl  2    5.6  1.0  26000
matl  3    1.0  2.0  1001  1.0 8016
matz  1   1 thru 16
matz  3  17 thru 32
reflx   33  34  35  36  37  38
source1  1  20.0  20.0   0.0
end
```

Planar Cell Example Input

```
name   reflector #4
box  t32
*
* Complete artificial planar cell example
*
critcalc  15  1  3.
zplane  1 -80.0
zplane  2 -40.0
zplane  3   0.0
zplane  4  40.0
zplane  5  80.0
yplane  6 -80.0
yplane 10  80.0
xplane 11 -20.0
xplane 12  20.0
zplane 13 -63.5
zplane 14 -56.5
zplane 15 -23.5
zplane 16 -16.5
zplane 17  16.5
zplane 18  23.5
zplane 19  56.5
zplane 20  63.5
* inside fuel
jb    1    -6 10 -11 12 -13 14
jb    2    -6 10 -11 12 -15 16
jb    3    -6 10 -11 12 -17 18
jb    4    -6 10 -11 12 -19 20
* inside water
jb    5    -6 10 -11 12  -1 13
jb    6    -6 10 -11 12 -14 15
jb    7    -6 10 -11 12 -16 17
jb    8    -6 10 -11 12 -18 19
jb   10    -6 10 -11 12 -20  5
* outside world
jb   33     1
jb   34    -5
jb   35     6
jb   36   -10
jb   37    11
jb   38   -12
matl 1   18.7 0.44 92235 0.56 92238
matl 2   5.6 1.0 26000
matl 3   1.0 2.0 1001 1.0 8016
```

```
matz  1   1 thru 4
matz  3   5 thru 10
reflx   33  34  35  36  37  38
source1  1   0.0   0.0  20.0
end
```